

Rigorous Solution of the Spin-1 Quantum Ising Model with Single-Ion Anisotropy

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We solve the spin-1 quantum Ising model with single-ion anisotropy by mapping it onto a series of segmented spin-1/2 transverse Ising chains, separated by the $S^z = 0$ states called holes. A recursion formula is derived for the partition function to simplify the summation of hole configurations. This allows the thermodynamic quantities of this model to be rigorously determined in the thermodynamic limit. The low temperature behavior is governed by the interplay between the hole excitations and the fermionic excitations within each spin-1/2 Ising segment. The quantum critical fluctuations around the Ising critical point of the transverse Ising model are strongly suppressed by the hole excitations.

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The quantum lattice models for which both the ground state and the finite temperature thermodynamics can be exactly solved are rare. However, these models play an important role in the study of quantum criticality. A typical example is the uniform $S = 1/2$ transverse Ising model (TIM), which sets a paradigm in elucidating the nature of both quantum and thermodynamic phase transitions [1–5]. Experimentally, this kind of lattice models can be realized in certain electronic materials [6–8] as well as in the optical lattice of cold atoms or polar molecules [9,10]. However, in many realistic situations, the local moments are larger than 1/2 and exposed to the interaction of single-ion anisotropy generated by the crystal fields [11]. In particular, in an integer spin system, a local spin can be in a neutral polarized states with $S^z = 0$. It is unclear how these extra degrees of freedom of spins can change the nature of quantum criticality revealed by the $S = 1/2$ TIM. To address unambiguously this problem, it is desired to find an extended but exactly soluble TIM model with higher spins.

In this Letter, we study an Ising model of $S = 1$ with the single-ion anisotropy, defined by the following Hamiltonian

$$H = - \sum_{j=1}^L [J S_j^z S_{j+1}^z + 2D_x (S_j^x)^2 + D_z (S_j^z)^2], \quad (1)$$

where L is the lattice length. In the classical limit, i.e., $D_x = 0$, it reduces to the Blume-Capel model [12,13]. The ground state of this model has been studied by a number of authors [14,15]. Oitmaa and Brasch first pointed out that in the ground state, this model is equivalent to the $S = 1/2$ TIM [15] and can therefore be exactly solved. Here, we want to show that the thermodynamic quantities of this model can be also rigorously calculated. To our knowledge, it is the first quantum $S = 1$ spin model whose thermodynamic properties can be rigorously studied without invoking the Bethe ansatz.

In Eq. (1), D_x and D_z are the coupling constants of the single-ion anisotropy along the x - and z -axes, respectively. A single-ion anisotropy along the y -axis can be added to this Hamiltonian. However, this term is not independent since $S^2 = 2$. It can be absorbed into the D_x and D_z terms. Equation (1) can be also extended to include the spin-1/2 magnetic impurities as well as longitude magnetic field. In the discussion below, free boundary conditions are assumed. It is straightforward to extend the results to the system with periodic boundary conditions.

At each site of the lattice, S_j^z can take three values, $S_j^z = 0, \pm 1$. Effectively, one can regard $S_j^z = \pm 1$ as the two polarized spin states of a $S = 1/2$ spin operator and $S_j^z = 0$ as a hole. A remarkable property of the Hamiltonian is that at each site, $(S_j^z)^2$ commutes with H . This means that the hole states ($S_j^z = 0$) are decoupled from the spin polarized states ($S_j^z = \pm 1$). Thus, the total number of holes is a good quantum number and can be used to classify the eigenstates of H .

The holes in this system act like nonmagnetic impurities. They will separate the system into many independent segments of interacting $S = 1/2$ spins. In a system of p holes, there are at most $p + 1$ segments of $S = 1/2$ spins. If these holes are located at $\{x_1, \dots, x_p\}$ with $1 \leq x_1 < \dots < x_p \leq L$, it is straightforward to show that Eq. (1) is exactly equivalent to the following Hamiltonian up to a dynamic irrelevant constant (setting $x_0 = 0$ and $x_{p+1} = L + 1$)

$$H(\{x_i, p\}) = \sum_{n=1}^{p+1} h(l_n) + p(D_z - D_x), \quad (2)$$

where

$$h(l_n) = - \sum_{j=x_{n-1}+1}^{x_n-2} J \sigma_j^z \sigma_{j+1}^z - \sum_{j=x_{n-1}+1}^{x_n-1} D_x \sigma_j^x, \quad (3)$$

$\sigma_\mu (\mu = x, z)$ are the Pauli matrices, and $l_n = x_n - x_{n-1} - 1$ is the segment length.

The above discussion indicates that in order to diagonalize the model, one needs only to diagonalize the Hamiltonian for each individual segment defined by Eq. (3). The eigenfunction of H is a product of all the eigenfunctions of the segment Hamiltonians $h(l_n)$. Correspondingly, the eigenvalue of H is simply given by the sum of the eigenvalues of $h(l_n)$. $D_z - D_x$ plays the role of chemical potential of holes. Thus, by adjusting the value of D_z , one can control the number of holes in the ground state.

$h(l)$ defined by Eq. (3) is the Hamiltonian of the $S = 1/2$ Ising model in a transverse field. It can be reduced to a model of noninteracting fermions by the Jordan-Wigner transformation. By further diagonalizing this fermionic model, the excitation spectrum can be obtained. The energy dispersion of the fermionic excitation is given by

$$\varepsilon(l) = \pm |D_x| \sqrt{1 + \lambda^2 + 2\lambda \cos k}, \quad (4)$$

where $\lambda = J/D_x$ and k is determined by the secular equation,

$$\frac{\sin(l+1)k}{\sin lk} = -\lambda. \quad (5)$$

This equation is reflection symmetric: if k is a solution, then $-k$ is also a solution. For $|\lambda| < 1$, k has $2l$ real roots within the interval $(-\pi, \pi]$. However, for $|\lambda| > 1$, k has $2l - 2$ real roots within $(-\pi, \pi]$ and two opposite complex roots. The eigenstates corresponding to these two complex solutions of k are two localized states, each trapped at one end of the chain.

The Hamiltonian (1) contains two kinds of excitations. One is the fermionic excitation within each segment, and the other is the hole excitations. The fermion excitation is gapped except at the critical point $|\lambda| = 1$. The minimal excitation gap is given by

$$\Delta_0 = 2|J| \left| \frac{1}{|\lambda|} - 1 \right|. \quad (6)$$

The minimal hole excitation gap is determined by the minimal energy for creating a hole at one end of the spin chain and given by

$$\Delta_h = E_0(L-1) - E_0(L) + D_z - D_x, \quad (7)$$

where $E_0(l)$ is the ground state energy of $h(l)$. Equation (7) holds when $\Delta_h > 0$. In the case $\Delta_h < 0$, holes will appear in the ground state. These holes will condense and break the system into many $S = 1/2$ spin segments. In this case, the hole excitation becomes gapless.

Figure 1 shows the λ dependence of the fermion and hole excitation gaps Δ_0 and Δ_h for $D_z = 0$. The spectrum of $h(L)$ is unchanged when λ changes to $-\lambda$. Thus, Δ_0 is symmetric under the reflection of λ . However, the hole excitation gap is nonsymmetric when λ changes to $-\lambda$.

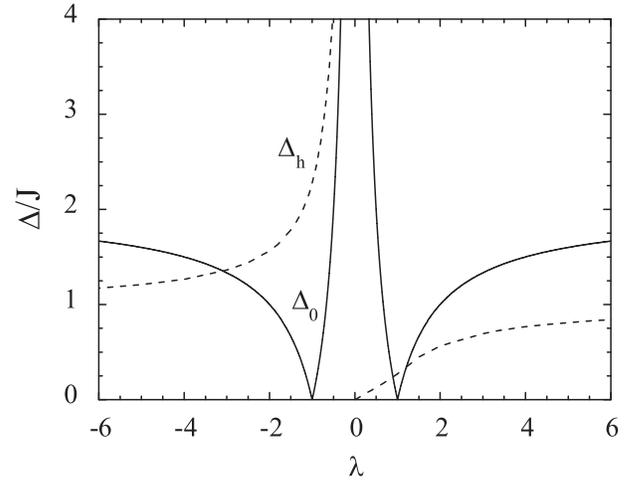


FIG. 1. Minimal energy for exciting a fermion quasiparticle Δ_0 or a hole Δ_h when $D_z = 0$.

When $\lambda > 0$, Δ_h is below Δ_0 except in a narrow region around the critical point $\lambda = 1$. At the critical point $\lambda = 1$, $\Delta_h = 0.273J$. In the case $\Delta_h < \Delta_0$, the low energy excitations are dominated by the hole excitations.

When $D_z = 0$, there is no hole in the ground state. In this case, the ground state can be either in a spin ordered phase at which all spins are either ferromagnetically or antiferromagnetically polarized along the z axis depending on the sign of J , or in a quantum disordered phase without any long-range spin order. The transition between these two phases at $|\lambda| = 1$ is of the Ising criticality.

Now let us consider the thermodynamic properties of the model. At first glance, it seems to be extremely difficult to calculate rigorously thermodynamic quantities of this system since the holes can take exponentially many configurations even though $h(l)$ can be analytically solved. However, for the system studied here, we find that the partition function can be expressed by the following recursion formula:

$$Z = \text{Tr} \exp(-\beta H) = \sum_{p=0}^L \alpha^p Z^{(p)}(L-p) \quad (8)$$

where $\alpha = \exp[\beta(D_x - D_z)]$ and

$$\begin{aligned} Z^{(p)}(l) &= \sum_{l_1 + \dots + l_{p+1} = l} z(l_1)z(l_2) \cdots z(l_{p+1}) \\ &= \sum_{l_1=0}^l z(l_1)Z^{(p-1)}(l-l_1). \end{aligned} \quad (9)$$

Here, we define $Z^{(0)}(l) = z(l) = \text{Tr} \exp[-\beta h(l)]$, $z(0) = 1$, and $z(1) = 2 \cosh(\beta D_x)$. Thus, the partition function can be evaluated recursively with Eq. (9), starting from a no-hole system. Given $z(l)$, the computing time needed just increases quadratically instead of exponentially with the lattice size. Therefore, this has greatly simplified the cal-

ulation. It allows us to access readily the thermodynamic limit by evaluating exactly the thermodynamic quantities in a sufficiently large lattice, for example $L = 10^4$, at which the finite size effect can be ignored.

From the partition function and its temperature derivatives, one can evaluate the free energy and all other thermodynamic quantities. One can also calculate directly the internal energy, the correlation functions, and other measurable variables from the corresponding segment quantities using the recursion formula of the partition function. For example, the internal energy is given by

$$U = \sum_{p=0}^L \alpha^p (p+1) \sum_{l=0}^{L-p} \frac{u(l)z(l)Z^{(p-1)}(L-p-l)}{Z(L)} + (D_z - D_x)N_h, \quad (10)$$

where, $Z^{(-1)}(l) \equiv \delta_{l,0}$, $u(l) = z^{-1}(l)\text{Tr}h(l)\exp[-\beta h(l)]$ is the internal energy of a segment, and N_h is the thermal average of the hole number defined by

$$N_h = \frac{1}{Z(L)} \sum_{p=0}^L p \alpha^p Z^{(p)}(L-p). \quad (11)$$

The specific heat can then be determined from the first order derivative of the internal energy.

Figure 2 shows the temperature dependence of the specific heat for several different λ and the temperature derivation of the hole excitation number. When $T \ll \min(\Delta_0, \Delta_h)$, the specific heat drops to zero exponentially with decreasing temperature, except at the quantum critical points. Above this exponential temperature dependent regime, two low temperature peaks appear in the specific heat curves when $0 < \lambda < 1.5$. These two peaks result from the hole and fermionic excitation and appear roughly at $T \sim \Delta_h$ and $T \sim \Delta_0$, respectively. This in fact can be more clearly seen from Fig. 2(b) where the temperature dependence of the specific heat for $\lambda = 0.5$ is shown and compared with the corresponding curve without any hole excitation $C(p=0)$ and with the temperature derivative of the thermal average number of holes dN_h/dT . For $\lambda = 0.5$, $\Delta_h < \Delta_0$, the low-lying excitations are dominated by the hole excitations. Thus the low temperature peak arises from the hole excitations.

When $D_z = 0$, there are no holes in the ground state. Thus, the quantum critical behavior of the model is not affected by the hole excitations at zero temperature. However, at finite temperature, the hole excitations can enhance the thermal fluctuation and suppress strongly the onset temperature T^* below which the quantum criticality is observed around the quantum critical point. Recently, Kopp and Chakravarty calculated the scaled free energy coefficient [5] for the $S = 1/2$ TIM

$$\Phi(T) = \frac{2|J|\sqrt{|\lambda|}[F(T) - F(0)]}{T^2}, \quad (12)$$

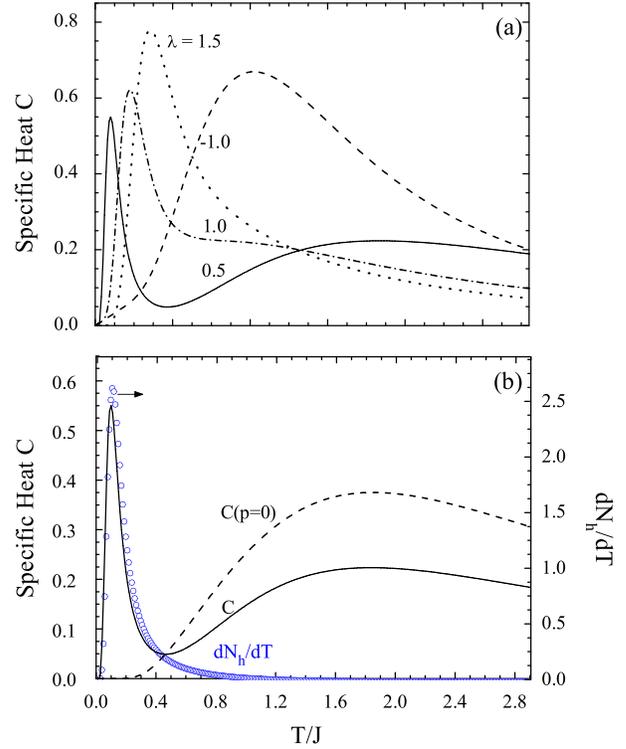


FIG. 2 (color online). Temperature dependence of (a) the specific heat C for several different λ and (b) the specific heat C and the temperature derivative of the hole excitation number dN_h/dT for the $S = 1$ Ising spin model (1) with $\lambda = 0.5$, $J = 1$, and $D_z = 0$. The specific heat for the same model but without hole excitations, $C(p=0)$, is also shown for comparison.

where $F(T)$ is the free energy, and the factor $2|J|\sqrt{|\lambda|}$ is the velocity of the elementary excitations ($\hbar = 1$) at low energy. At the critical point, $\lambda = 1$, they found that $\Phi(T)$ already falls into the quantum critical scaling regime with $\Phi(T) \approx \Phi(0) = \pi/12$ at $T^* \leq J/2$. This suggests that the quantum criticality in the $S = 1/2$ TIM can persist up to a surprisingly high temperature. However, in the presence of holes, we find that the persistence of the quantum critical behavior of the system is modified. Figure 3 shows Φ as a function of J/T for the $S = 1$ TIM at the two critical points ($\lambda = \pm 1$) and compared with the corresponding results for the $S = 1/2$ TIM. In the case $\lambda = 1$, Φ shows a broad peak around $T \sim J/2$, and the onset temperature T^* of quantum criticality is suppressed by nearly 1 order of magnitude due to the hole excitations. However, at $\lambda = -1$, the suppression is relatively weak since the hole excitation gap is much larger than $J/2$.

When the hole excitation has a finite energy gap, the ground state is magnetically disordered when $|\lambda| < 1$ but ordered (either ferromagnetic or antiferromagnetic, depending on the sign of J) when $|\lambda| > 1$. However, for sufficiently large but negative D_z, Δ_h defined by Eq. (7) becomes negative. In this case, the static holes will condense in low temperatures. Figure 4(a) shows the ground

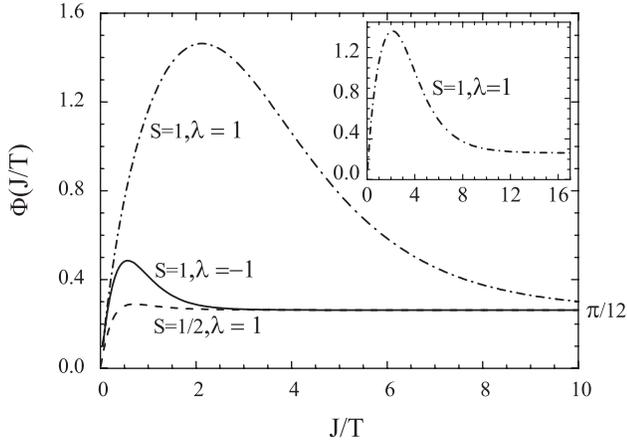


FIG. 3. The temperature dependence of $\Phi(T)$. The inset shows $\Phi(T)$ versus J/T for $\lambda = 1$ and $S = 1$ in a wider temperature range.

state phase diagram. Across the hole condensed phase boundary, both the magnetization m and the hole excitation number N_h , as shown in Figs. 4(b) and 4(c), change discontinuously at zero temperature. This is a typical characteristic of the first order phase transition.

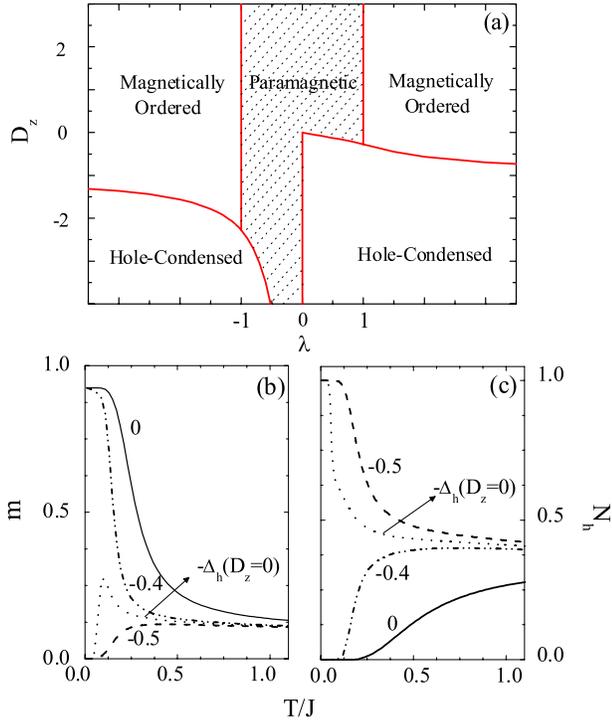


FIG. 4 (color online). (a) The phase diagram of the ground state. (b) and (c) show the temperature dependence of the magnetization $m = \sqrt{\sum_{ij} \langle S_i^z S_j^z \rangle} / L$ and the corresponding hole excitation number N_h for several D_z with $J = 1$, $\lambda = 1.5$, and $\Delta_h(D_z = 0) = 0.447974J$.

In summary, we have developed a recursive method to solve the thermodynamics of the $S = 1$ quantum Ising chain with single-ion anisotropy. This allows us to evaluate rigorously all thermodynamic quantities in the thermodynamic limit. The hole excitations affect strongly the low temperature behaviors of the system. They enhance the thermodynamic fluctuations and reduce strongly the characteristic temperature of quantum criticality. The formulas derived in this work hold not just for the model studied here. With proper extension, they can also be applied to study thermodynamic properties of quasi-one-dimensional antiferromagnets with nonmagnetic impurities, such as $\text{Sr}_2(\text{Cu}_{1-x}\text{Pd}_x)\text{O}_3$ [16,17], $\text{Cu}_{1-x}\text{Zn}_x\text{GeO}_3$ [18], as well as other physical systems whose Hamiltonian can be written as a sum of independent spin segments, separated by nonmagnetic impurities.

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